



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2020 – 09:45 AM BST

PDB ID : 4P00
Title : Bacterial Cellulose Synthase in complex with cyclic-di-GMP and UDP
Authors : Morgan, J.L.W.; McNamara, J.T.; Zimmer, J.
Deposited on : 2014-02-19
Resolution : 3.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

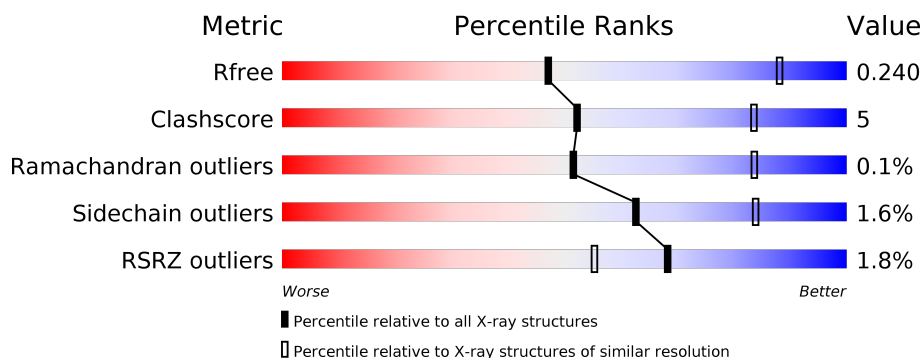
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	803	<div> <div>2%</div> <div> <div></div> <div>77%</div> <div>13%</div> <div>9%</div> </div> </div>
2	B	724	<div> <div>%</div> <div> <div></div> <div>78%</div> <div>12%</div> <div>10%</div> </div> </div>
3	D	9	<div> <div></div> <div>100%</div> </div>
4	C	17	<div> <div>29%</div> <div>47%</div> <div>24%</div> </div>

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 11070 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Cellulose Synthase A subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	728	Total	C	N	O	S	0	1	0
			5739	3725	1000	982	32			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	expression tag	UNP Q3J125
A	1	GLY	-	expression tag	UNP Q3J125
A	789	HIS	-	expression tag	UNP Q3J125
A	790	HIS	-	expression tag	UNP Q3J125
A	791	HIS	-	expression tag	UNP Q3J125
A	792	HIS	-	expression tag	UNP Q3J125
A	793	HIS	-	expression tag	UNP Q3J125
A	794	HIS	-	expression tag	UNP Q3J125
A	795	LYS	-	expression tag	UNP Q3J125
A	796	LEU	-	expression tag	UNP Q3J125
A	797	HIS	-	expression tag	UNP Q3J125
A	798	HIS	-	expression tag	UNP Q3J125
A	799	HIS	-	expression tag	UNP Q3J125
A	800	HIS	-	expression tag	UNP Q3J125
A	801	HIS	-	expression tag	UNP Q3J125
A	802	HIS	-	expression tag	UNP Q3J125

- Molecule 2 is a protein called Cellulose Synthase B subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	655	Total	C	N	O	S	0	5	0
			4923	3120	872	915	16			

- Molecule 3 is a protein called unidentified peptide.

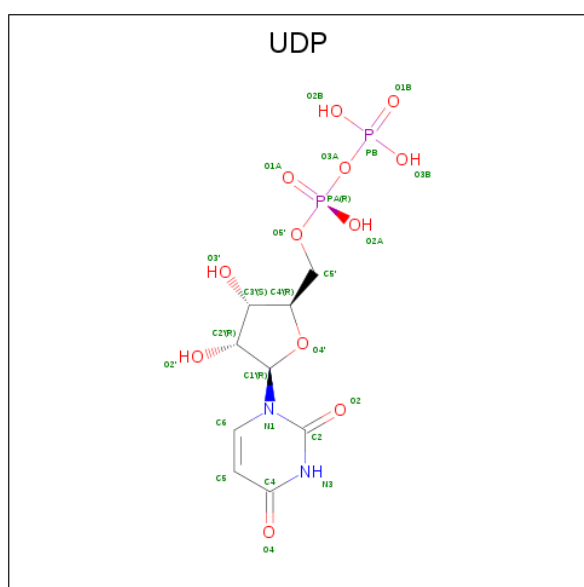
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	D	9	Total	C	N	O	0	0	0
			45	27	9	9			

- [illegible]



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
4	C	17	Total C O 187 102 85	0	0	0

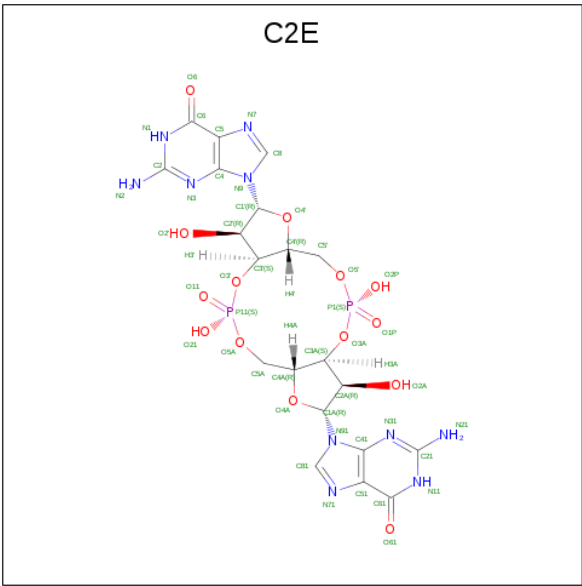
- Molecule 5 is URIDINE-5'-DIPHOSPHATE (three-letter code: UDP) (formula: $\text{C}_9\text{H}_{14}\text{N}_2\text{O}_{12}\text{P}_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			25	9	2	12	2		

- Molecule 6 is 9,9'-[(2R,3R,3aS,5S,7aR,9R,10R,10aS,12S,14aR)-3,5,10,12-tetrahydro-5,12-dioxidoctahydro-2H,7H-difuro[3,2-d:3',2'-j][1,3,7,9,2,8]tetraoxadiphosphacyclododecine-2,9-diyl]bis(2-amino-1,9-dihydro-6H-purin-6-one) (three-letter code: C2E) (formula:

C₂₀H₂₄N₁₀O₁₄P₂).

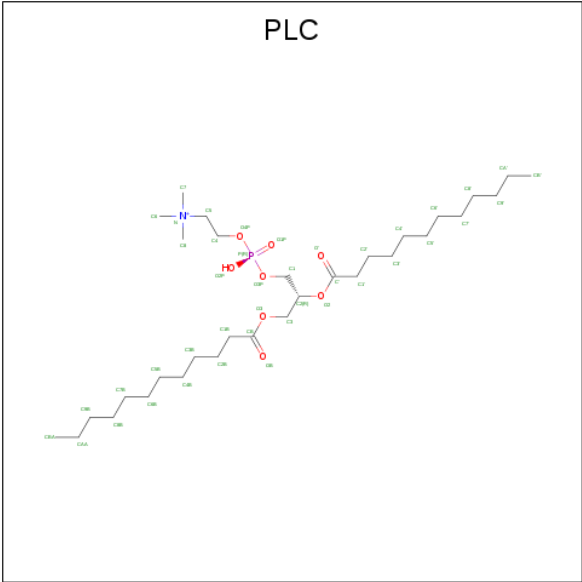


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total 46	C 20	N 10	O 14	P 2	0	0
6	A	1	Total 46	C 20	N 10	O 14	P 2	0	0

- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

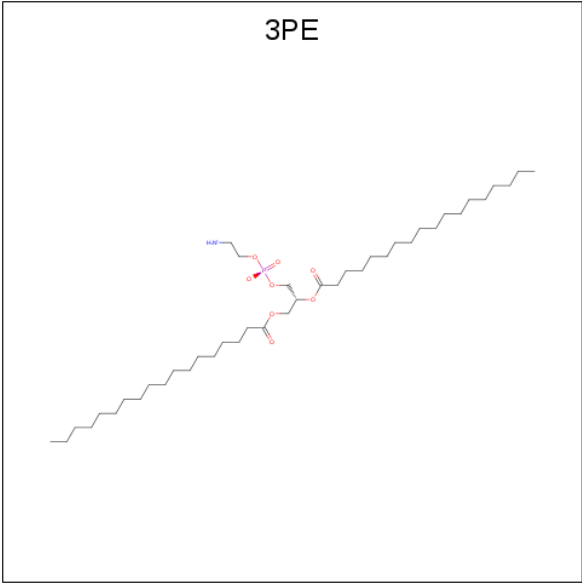
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Mg	0	0
			1	1		

- Molecule 8 is DIUNDECYL PHOSPHATIDYL CHOLINE (three-letter code: PLC) (formula: C₃₂H₆₅N₁O₈P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	A	1	Total	C	N	O	P	0	0
			38	28	1	8	1		

- Molecule 9 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOETHANOLAMINE (three-letter code: 3PE) (formula: $C_{41}H_{82}NO_8P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	A	1	Total	C	N	O	P	0	0
			20	10	1	8	1		

- Molecule 1: Cellulose Synthase A subunit





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	67.49 Å 216.79 Å 219.62 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.98 – 3.20 49.62 – 3.20	Depositor EDS
% Data completeness (in resolution range)	98.2 (48.98-3.20) 98.2 (49.62-3.20)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.45 (at 3.19 Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, R_{free}	0.208 , 0.238 0.214 , 0.240	Depositor DCC
R_{free} test set	2716 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å ²)	70.0	Xtriage
Anisotropy	0.491	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 39.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.017 for -h,l,k	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	11070	wwPDB-VP
Average B, all atoms (Å ²)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.73% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: UDP, BGC, MG, PLC, C2E, 3PE

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.21	0/5888	0.37	0/8007
2	B	0.20	0/5042	0.40	0/6913
All	All	0.21	0/10930	0.38	0/14920

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5739	0	5855	64	0
2	B	4923	0	4997	51	0
3	D	45	0	12	0	0
4	C	187	0	154	9	0
5	A	25	0	11	1	0
6	A	92	0	44	11	0
7	A	1	0	0	0	0
8	A	38	0	53	1	0
9	A	20	0	14	1	0
All	All	11070	0	11140	122	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including

hydrogen atoms). The all-atom clashscore for this structure is 5.

All (122) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:920:C2E:H81	6:A:920:C2E:H511	1.21	1.11
6:A:920:C2E:H81	6:A:920:C2E:C5A	1.93	0.98
1:A:578:GLN:OE1	6:A:920:C2E:N2	1.99	0.94
2:B:390:ARG:NH2	4:C:5:BGC:O6	2.05	0.88
1:A:57:LYS:NZ	9:A:923:3PE:O12	2.16	0.78
1:A:578:GLN:OE1	6:A:920:C2E:N1	2.20	0.74
4:C:4:BGC:O3	4:C:5:BGC:O5	2.06	0.73
1:A:578:GLN:OE1	6:A:920:C2E:C2	2.40	0.69
1:A:311:ARG:HH22	2:B:719:THR:HG23	1.59	0.68
1:A:312:TRP:HB3	1:A:405:ALA:HB1	1.80	0.63
1:A:42:GLN:OE1	1:A:79:ARG:NH1	2.32	0.63
1:A:385:THR:HG23	1:A:494:THR:HG21	1.80	0.63
1:A:419:PHE:HA	1:A:422:VAL:HG22	1.82	0.61
4:C:5:BGC:O3	4:C:6:BGC:O5	2.16	0.61
6:A:920:C2E:C81	6:A:920:C2E:H511	2.14	0.61
1:A:35:ALA:O	1:A:79:ARG:NH2	2.34	0.60
2:B:77[A]:GLN:HG3	2:B:157:HIS:H	1.67	0.59
2:B:377:LYS:HB2	2:B:416:SER:HB2	1.85	0.59
1:A:300:MET:HA	1:A:470:GLN:HB3	1.85	0.58
2:B:425:PRO:HG2	2:B:428:GLN:HB2	1.86	0.58
2:B:270:ILE:HG22	2:B:280:LEU:HA	1.85	0.58
1:A:432:ILE:HD11	1:A:440:ILE:HD13	1.85	0.58
2:B:360:ILE:HA	2:B:444:THR:HG23	1.85	0.57
2:B:328:THR:HG22	2:B:442:SER:H	1.69	0.57
4:C:4:BGC:HC	4:C:5:BGC:C5	2.16	0.57
2:B:693:ARG:HG2	2:B:695:PRO:HD2	1.85	0.57
2:B:358:ILE:HG12	2:B:446:LEU:HD23	1.87	0.56
1:A:343:ASP:N	1:A:343:ASP:OD1	2.38	0.56
2:B:320:THR:HA	2:B:445:ASP:HA	1.86	0.56
2:B:59:LEU:HD13	2:B:85:LEU:HD13	1.86	0.56
1:A:480:GLU:OE2	4:C:14:BGC:O6	2.21	0.55
1:A:654:ARG:O	1:A:677:GLN:NE2	2.39	0.55
1:A:161:ALA:HB1	1:A:683:GLU:HG2	1.88	0.55
1:A:394:LYS:O	1:A:399:ARG:NH1	2.40	0.55
1:A:372:THR:HG22	1:A:512:LEU:HD21	1.90	0.54
1:A:151:GLU:O	1:A:201:ARG:NH2	2.42	0.53
2:B:185:PRO:HG2	2:B:188:ALA:HB2	1.89	0.53
2:B:101:ARG:NE	2:B:174:GLU:OE1	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:349:GLU:OE2	1:A:399:ARG:NH2	2.42	0.52
1:A:66:ARG:NH1	1:A:123:ALA:O	2.42	0.52
1:A:547:GLY:O	4:C:7:BGC:O6	2.27	0.52
1:A:84:ARG:NH1	1:A:108:GLU:OE1	2.42	0.52
2:B:475:THR:HG22	2:B:477:ASP:H	1.73	0.52
2:B:606:THR:HG23	2:B:607:ARG:HE	1.74	0.51
1:A:219:ARG:HD3	1:A:229:ASN:HA	1.93	0.51
1:A:57:LYS:HG3	1:A:465:ALA:HB2	1.92	0.51
1:A:587:MET:N	1:A:608:LEU:O	2.41	0.51
2:B:287:GLU:OE1	2:B:287:GLU:N	2.44	0.51
6:A:919:C2E:H2'	6:A:920:C2E:N11	2.26	0.50
1:A:296:PRO:HG2	1:A:299:GLU:HB2	1.93	0.50
1:A:446:GLU:OE2	2:B:573:ARG:NH2	2.41	0.50
1:A:402:LEU:O	1:A:407:ARG:NH2	2.45	0.49
1:A:274:THR:OG1	1:A:321:ALA:O	2.21	0.49
1:A:183:THR:H	1:A:186:ARG:HB2	1.78	0.49
1:A:276:HIS:O	1:A:298:ASN:ND2	2.46	0.49
1:A:515:ASN:OD1	1:A:577:GLN:N	2.46	0.49
2:B:57:ILE:HD13	2:B:184:LEU:HD21	1.95	0.48
1:A:482:ALA:HB2	1:A:569:ALA:HB1	1.95	0.47
1:A:272:VAL:HG22	1:A:358:LEU:HD21	1.96	0.47
1:A:369:GLN:HG3	1:A:370:PRO:HD2	1.96	0.47
1:A:580:ARG:NH2	6:A:920:C2E:H2'	2.31	0.46
1:A:534:GLY:O	1:A:538:THR:HG23	2.16	0.46
1:A:579:ARG:O	6:A:919:C2E:H5'1	2.15	0.46
1:A:419:PHE:CD2	1:A:420:PRO:HD3	2.50	0.46
1:A:382:ARG:NH2	5:A:918:UDP:O2A	2.49	0.46
8:A:922:PLC:H71	4:C:6:BGC:O3	2.16	0.46
1:A:152:PRO:HB2	1:A:154:ASP:OD1	2.16	0.46
2:B:78[A]:GLN:HE21	2:B:333:ASN:HD21	1.63	0.46
1:A:29:PHE:HZ	1:A:75:MET:HA	1.80	0.46
2:B:77[A]:GLN:HE22	2:B:158:ARG:CZ	2.28	0.46
2:B:396:LYS:HG3	2:B:397:PRO:HD2	1.97	0.46
1:A:607:VAL:HG13	1:A:615:VAL:HG13	1.98	0.45
1:A:394:LYS:HA	1:A:394:LYS:HD3	1.75	0.45
1:A:616:ARG:HB2	6:A:919:C2E:HN11	1.81	0.45
2:B:103:SER:HB2	2:B:172:TRP:CD2	2.52	0.45
2:B:200:LEU:HD13	2:B:239:LEU:HD21	1.98	0.45
2:B:148:ASP:HB3	2:B:305:LEU:HG	1.98	0.45
2:B:350:LEU:HD23	2:B:354:GLN:HB2	1.99	0.45
2:B:78[A]:GLN:HE21	2:B:333:ASN:ND2	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:74:SER:HA	1:A:77:VAL:HG22	1.99	0.45
1:A:243:VAL:HG22	1:A:323:VAL:HG12	2.00	0.44
2:B:285:PRO:HA	2:B:286:PRO:HD3	1.90	0.44
2:B:272:ARG:NH2	2:B:276:GLY:O	2.44	0.44
1:A:203:ARG:NH1	1:A:207:GLN:HB2	2.33	0.43
1:A:144:ILE:HG13	1:A:243:VAL:HB	2.00	0.43
2:B:310:LEU:HB2	2:B:343:GLN:HG2	1.99	0.43
1:A:392:LEU:HD11	1:A:495:LEU:HD23	2.00	0.43
6:A:920:C2E:C5A	6:A:920:C2E:C81	2.82	0.43
2:B:261:LEU:HD12	2:B:262:PRO:HD2	2.01	0.43
4:C:1:BGC:H6C1	4:C:2:BGC:O2	2.19	0.43
1:A:389:GLN:NE2	1:A:498:PRO:O	2.51	0.43
2:B:234:LEU:HD12	2:B:239:LEU:HD11	2.01	0.43
2:B:70:PRO:HG2	2:B:71:LEU:HD12	2.01	0.43
2:B:262:PRO:HB3	2:B:286:PRO:HG3	2.01	0.43
2:B:117:MET:HE2	2:B:122:ILE:HG21	2.01	0.42
2:B:641:ALA:HB1	2:B:648:PRO:HD2	2.01	0.42
1:A:384:ALA:O	1:A:388:MET:HG2	2.20	0.42
2:B:73:ARG:NH1	2:B:174:GLU:OE2	2.53	0.42
1:A:387:MET:HG3	1:A:417:TRP:CD1	2.54	0.42
2:B:157:HIS:CE1	2:B:173:THR:HG22	2.55	0.42
1:A:147:PRO:HG3	1:A:230:MET:HE3	2.01	0.42
2:B:350:LEU:HD21	2:B:449:PRO:HB2	2.02	0.42
2:B:55:TRP:CE3	2:B:189:ILE:HG13	2.54	0.41
2:B:266:ASP:OD1	2:B:266:ASP:N	2.53	0.41
1:A:464:ASN:O	1:A:468:ALA:HB2	2.19	0.41
2:B:369:PRO:HB2	2:B:422:PRO:HG2	2.02	0.41
1:A:441:PHE:HB3	4:C:9:BGC:O4	2.21	0.41
1:A:40:SER:HA	2:B:581:THR:HG22	2.02	0.41
2:B:307:PRO:HA	2:B:308:PRO:HD3	1.91	0.41
1:A:184:ASP:HB2	1:A:220:GLU:HA	2.03	0.41
2:B:76[A]:GLY:HA2	2:B:168:GLU:O	2.20	0.41
1:A:448:VAL:O	1:A:453:PRO:HD3	2.20	0.41
2:B:238:ALA:HB2	2:B:488:ALA:HB2	2.03	0.41
1:A:218:THR:OG1	1:A:219:ARG:N	2.54	0.41
2:B:267:ARG:HG2	2:B:283:GLU:HB2	2.03	0.41
1:A:677:GLN:HB3	1:A:681:VAL:HG21	2.03	0.41
2:B:263:SER:OG	2:B:264:ASP:N	2.50	0.41
1:A:271:LEU:HD11	1:A:317:PHE:HB2	2.02	0.40
2:B:425:PRO:HA	2:B:426:PRO:HD3	1.85	0.40
2:B:678:SER:O	2:B:682:VAL:HG23	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:595:ILE:HG12	1:A:637:ILE:HG13	2.02	0.40
2:B:321:LEU:HB3	2:B:326:VAL:HG22	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	727/803 (90%)	689 (95%)	36 (5%)	2 (0%)	41	74
2	B	656/724 (91%)	632 (96%)	24 (4%)	0	100	100
All	All	1383/1527 (91%)	1321 (96%)	60 (4%)	2 (0%)	51	83

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	574	ALA
1	A	167	ILE

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	599/661 (91%)	591 (99%)	8 (1%)	69	87
2	B	523/572 (91%)	513 (98%)	10 (2%)	57	81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1122/1233 (91%)	1104 (98%)	18 (2%)	62 84

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	VAL
1	A	175	VAL
1	A	341	THR
1	A	358	LEU
1	A	369	GLN
1	A	446	GLU
1	A	568	PHE
1	A	627	PRO
2	B	87	LEU
2	B	144	VAL
2	B	148	ASP
2	B	266	ASP
2	B	326	VAL
2	B	378	VAL
2	B	523	LEU
2	B	575	GLN
2	B	643	ARG
2	B	672	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

17 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	BGC	C	1	4	11,11,12	0.30	0	15,15,17	0.82	0
4	BGC	C	10	4	11,11,12	0.32	0	15,15,17	0.88	1 (6%)
4	BGC	C	11	4	11,11,12	0.29	0	15,15,17	0.70	0
4	BGC	C	12	4	11,11,12	0.30	0	15,15,17	0.83	1 (6%)
4	BGC	C	13	4	11,11,12	0.30	0	15,15,17	0.67	0
4	BGC	C	14	4	11,11,12	0.33	0	15,15,17	1.34	1 (6%)
4	BGC	C	15	4	11,11,12	0.31	0	15,15,17	0.89	1 (6%)
4	BGC	C	16	4	11,11,12	0.29	0	15,15,17	0.76	0
4	BGC	C	17	4	11,11,12	0.25	0	15,15,17	0.71	0
4	BGC	C	2	4	11,11,12	0.34	0	15,15,17	0.93	0
4	BGC	C	3	4	11,11,12	0.30	0	15,15,17	0.82	0
4	BGC	C	4	4	11,11,12	0.38	0	15,15,17	1.26	1 (6%)
4	BGC	C	5	4	11,11,12	0.44	0	15,15,17	1.63	2 (13%)
4	BGC	C	6	4	11,11,12	0.26	0	15,15,17	0.70	0
4	BGC	C	7	4	11,11,12	0.27	0	15,15,17	0.95	1 (6%)
4	BGC	C	8	4	11,11,12	0.37	0	15,15,17	1.16	1 (6%)
4	BGC	C	9	4	11,11,12	0.30	0	15,15,17	0.76	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	BGC	C	1	4	-	0/2/19/22	0/1/1/1
4	BGC	C	10	4	-	1/2/19/22	0/1/1/1
4	BGC	C	11	4	-	0/2/19/22	0/1/1/1
4	BGC	C	12	4	-	0/2/19/22	0/1/1/1
4	BGC	C	13	4	-	0/2/19/22	0/1/1/1
4	BGC	C	14	4	-	0/2/19/22	0/1/1/1
4	BGC	C	15	4	-	0/2/19/22	0/1/1/1
4	BGC	C	16	4	-	1/2/19/22	0/1/1/1
4	BGC	C	17	4	-	0/2/19/22	0/1/1/1
4	BGC	C	2	4	-	1/2/19/22	0/1/1/1
4	BGC	C	3	4	-	1/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	BGC	C	4	4	-	0/2/19/22	0/1/1/1
4	BGC	C	5	4	-	1/2/19/22	0/1/1/1
4	BGC	C	6	4	-	2/2/19/22	0/1/1/1
4	BGC	C	7	4	-	2/2/19/22	0/1/1/1
4	BGC	C	8	4	-	0/2/19/22	0/1/1/1
4	BGC	C	9	4	-	2/2/19/22	0/1/1/1

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	5	BGC	C1-C2-C3	4.50	115.20	109.67
4	C	14	BGC	C1-C2-C3	4.17	114.79	109.67
4	C	4	BGC	C1-C2-C3	3.71	114.23	109.67
4	C	10	BGC	C1-C2-C3	2.66	112.93	109.67
4	C	5	BGC	C2-C3-C4	2.54	115.28	110.89
4	C	7	BGC	O5-C1-C2	-2.39	107.08	110.77
4	C	8	BGC	C3-C4-C5	2.28	114.30	110.24
4	C	12	BGC	C1-C2-C3	2.24	112.42	109.67
4	C	15	BGC	O5-C1-C2	-2.16	107.44	110.77

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	6	BGC	O5-C5-C6-O6
4	C	6	BGC	C4-C5-C6-O6
4	C	9	BGC	O5-C5-C6-O6
4	C	9	BGC	C4-C5-C6-O6
4	C	7	BGC	O5-C5-C6-O6
4	C	10	BGC	O5-C5-C6-O6
4	C	3	BGC	O5-C5-C6-O6
4	C	5	BGC	O5-C5-C6-O6
4	C	16	BGC	O5-C5-C6-O6
4	C	2	BGC	O5-C5-C6-O6
4	C	7	BGC	C4-C5-C6-O6

There are no ring outliers.

8 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	2	BGC	1	0
4	C	5	BGC	4	0
4	C	14	BGC	1	0
4	C	6	BGC	2	0
4	C	9	BGC	1	0
4	C	7	BGC	1	0
4	C	4	BGC	2	0
4	C	1	BGC	1	0

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 1 is monoatomic - leaving 5 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
6	C2E	A	920	-	44,52,52	1.21	4 (9%)	54,82,82	1.87	13 (24%)
9	3PE	A	923	-	19,19,50	1.58	2 (10%)	22,24,55	1.64	3 (13%)
5	UDP	A	918	7	20,26,26	1.11	1 (5%)	25,40,40	1.21	2 (8%)
8	PLC	A	922	-	37,37,41	1.12	2 (5%)	43,45,49	1.10	3 (6%)
6	C2E	A	919	-	44,52,52	1.23	4 (9%)	54,82,82	1.88	13 (24%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	C2E	A	920	-	-	12/22/62/62	0/6/7/7
9	3PE	A	923	-	-	4/22/22/54	-
5	UDP	A	918	7	-	6/14/32/32	0/2/2/2
8	PLC	A	922	-	-	22/41/41/45	-
6	C2E	A	919	-	-	7/22/62/62	0/6/7/7

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	923	3PE	O21-C21	4.71	1.45	1.35
9	A	923	3PE	O31-C31	4.31	1.45	1.33
8	A	922	PLC	O3-CB	4.30	1.45	1.33
6	A	919	C2E	C61-C51	4.26	1.48	1.41
6	A	920	C2E	C6-C5	4.24	1.48	1.41
6	A	919	C2E	C6-C5	4.15	1.48	1.41
8	A	922	PLC	O2-C'	4.13	1.46	1.34
6	A	920	C2E	C61-C51	4.11	1.48	1.41
5	A	918	UDP	C4-N3	3.03	1.38	1.33
6	A	920	C2E	C5-C4	2.42	1.47	1.40
6	A	920	C2E	C51-C41	2.40	1.47	1.40
6	A	919	C2E	C5-C4	2.37	1.47	1.40
6	A	919	C2E	C51-C41	2.35	1.47	1.40

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	923	3PE	O21-C21-C22	5.00	120.29	111.09
6	A	920	C2E	C21-N31-C41	4.90	120.96	115.36
6	A	919	C2E	C21-N31-C41	4.78	120.82	115.36
6	A	920	C2E	C2-N3-C4	4.74	120.77	115.36
6	A	919	C2E	C2-N3-C4	4.74	120.77	115.36
8	A	922	PLC	O2-C'-C1'	4.08	120.30	111.50
6	A	919	C2E	C5-C6-N1	-3.90	118.10	123.43
6	A	920	C2E	C5-C6-N1	-3.90	118.10	123.43
6	A	919	C2E	C51-C61-N11	-3.89	118.11	123.43
6	A	919	C2E	C61-C51-C41	-3.85	117.12	120.80
6	A	919	C2E	C61-N11-C21	3.81	121.98	115.93
6	A	920	C2E	C51-C61-N11	-3.79	118.25	123.43
6	A	920	C2E	C6-N1-C2	3.78	121.93	115.93
6	A	919	C2E	C6-N1-C2	3.76	121.91	115.93
6	A	920	C2E	C6-C5-C4	-3.74	117.22	120.80
6	A	920	C2E	C61-N11-C21	3.74	121.86	115.93
6	A	920	C2E	C61-C51-C41	-3.68	117.29	120.80
6	A	919	C2E	C6-C5-C4	-3.64	117.32	120.80
5	A	918	UDP	PA-O3A-PB	-3.54	120.68	132.83
9	A	923	3PE	O31-C31-C32	3.32	120.10	111.38
6	A	920	C2E	N31-C21-N11	-3.09	123.09	127.22
6	A	919	C2E	N31-C21-N11	-3.08	123.11	127.22
9	A	923	3PE	C2-O21-C21	-3.07	112.18	117.90
6	A	919	C2E	N3-C2-N1	-3.01	123.20	127.22
6	A	920	C2E	N3-C2-N1	-2.99	123.23	127.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	920	C2E	C4-C5-N7	-2.91	106.37	109.40
6	A	919	C2E	C41-C51-N71	-2.83	106.45	109.40
6	A	919	C2E	C4-C5-N7	-2.73	106.55	109.40
6	A	920	C2E	C41-C51-N71	-2.73	106.56	109.40
8	A	922	PLC	O3-CB-C1B	2.67	120.30	111.91
5	A	918	UDP	C3'-C2'-C1'	2.57	104.85	100.98
6	A	919	C2E	C3'-C2'-C1'	2.43	105.27	99.89
6	A	920	C2E	C3'-C2'-C1'	2.34	105.08	99.89
8	A	922	PLC	C2-O2-C'	-2.24	112.28	117.79

There are no chirality outliers.

All (51) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	922	PLC	O4P-C4-C5-N
8	A	922	PLC	C5-C4-O4P-P
8	A	922	PLC	C4-O4P-P-O1P
6	A	919	C2E	C5'-O5'-P1-O1P
6	A	920	C2E	C5'-O5'-P1-O1P
6	A	920	C2E	O4'-C4'-C5'-O5'
6	A	920	C2E	C5A-O5A-P11-O3'
6	A	920	C2E	C5A-O5A-P11-O21
6	A	920	C2E	C5A-O5A-P11-O11
5	A	918	UDP	C5'-O5'-PA-O3A
9	A	923	3PE	O32-C31-O31-C3
9	A	923	3PE	C32-C31-O31-C3
6	A	920	C2E	C3'-C4'-C5'-O5'
6	A	920	C2E	O4A-C4A-C5A-O5A
8	A	922	PLC	C1B-CB-O3-C3
8	A	922	PLC	CB-C1B-C2B-C3B
8	A	922	PLC	OB-CB-O3-C3
6	A	919	C2E	C2'-C3'-O3'-P11
6	A	920	C2E	C5'-O5'-P1-O3A
8	A	922	PLC	C5B-C6B-C7B-C8B
8	A	922	PLC	C1'-C2'-C3'-C4'
6	A	919	C2E	C4'-C3'-O3'-P11
8	A	922	PLC	C6B-C7B-C8B-C9B
6	A	920	C2E	C3A-C4A-C5A-O5A
5	A	918	UDP	O4'-C4'-C5'-O5'
8	A	922	PLC	C1'-C'-O2-C2
8	A	922	PLC	C8B-C9B-CAA-CBA
5	A	918	UDP	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
8	A	922	PLC	O3P-C1-C2-O2
8	A	922	PLC	C7B-C8B-C9B-CAA
8	A	922	PLC	O3P-C1-C2-C3
8	A	922	PLC	O'-C'-O2-C2
6	A	920	C2E	C3A-O3A-P1-O2P
8	A	922	PLC	C1B-C2B-C3B-C4B
6	A	919	C2E	O4'-C4'-C5'-O5'
8	A	922	PLC	C4-O4P-P-O3P
6	A	919	C2E	C5'-O5'-P1-O3A
6	A	919	C2E	C5'-O5'-P1-O2P
6	A	920	C2E	C5'-O5'-P1-O2P
5	A	918	UDP	C5'-O5'-PA-O1A
5	A	918	UDP	C5'-O5'-PA-O2A
8	A	922	PLC	C4'-C5'-C6'-C7'
9	A	923	3PE	C1-O11-P-O13
6	A	919	C2E	C3'-C4'-C5'-O5'
8	A	922	PLC	C'-C1'-C2'-C3'
6	A	920	C2E	C3A-O3A-P1-O5'
8	A	922	PLC	C2B-C3B-C4B-C5B
5	A	918	UDP	PB-O3A-PA-O1A
9	A	923	3PE	C1-O11-P-O14
8	A	922	PLC	C3B-C4B-C5B-C6B
8	A	922	PLC	C2'-C3'-C4'-C5'

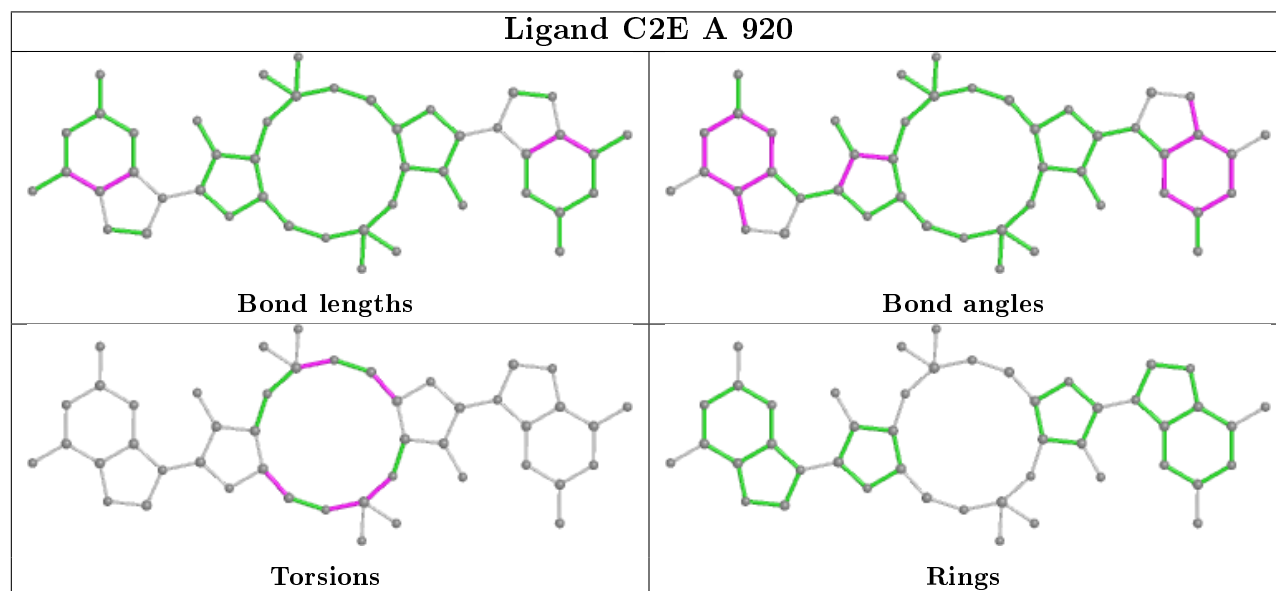
There are no ring outliers.

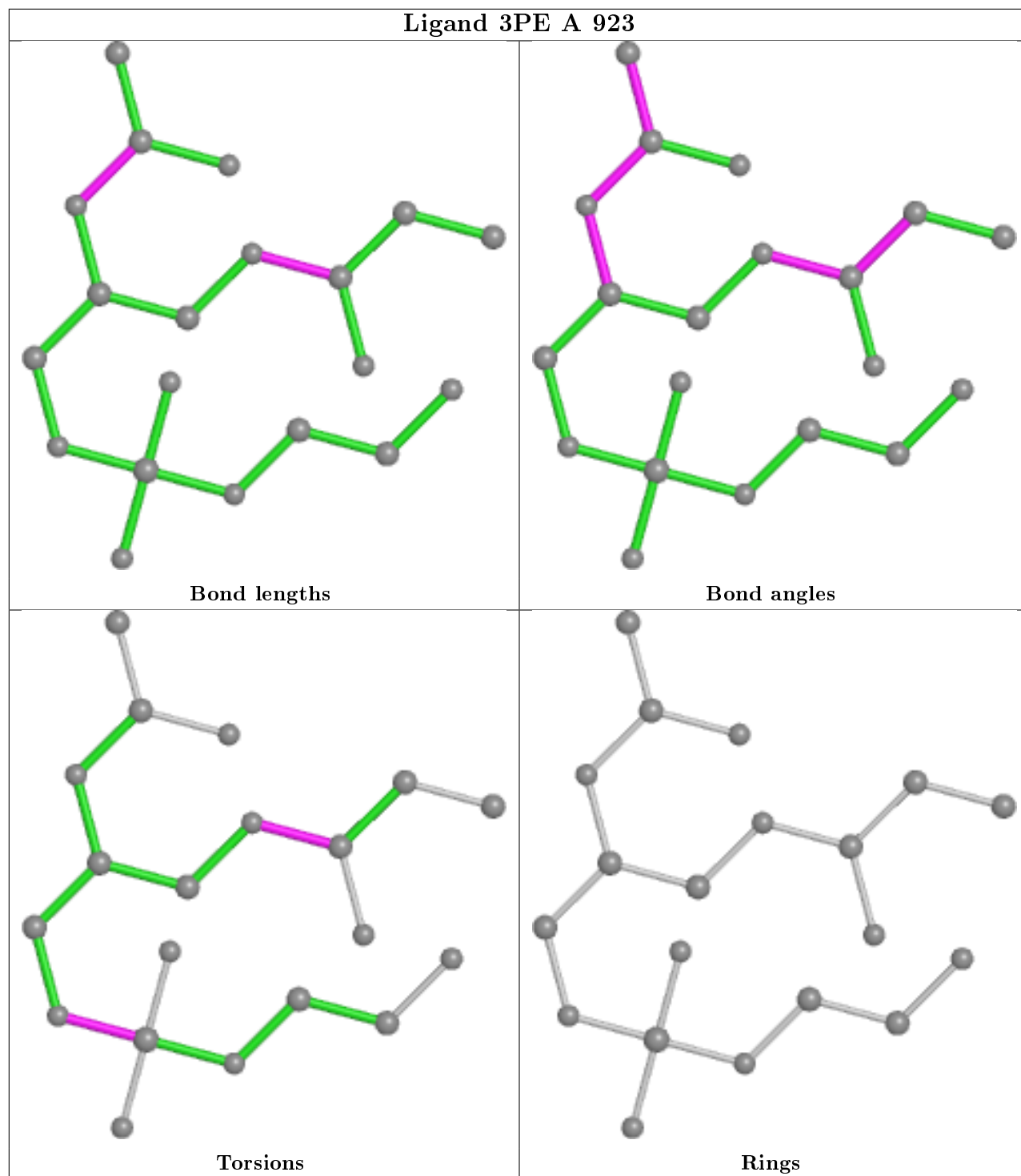
5 monomers are involved in 14 short contacts:

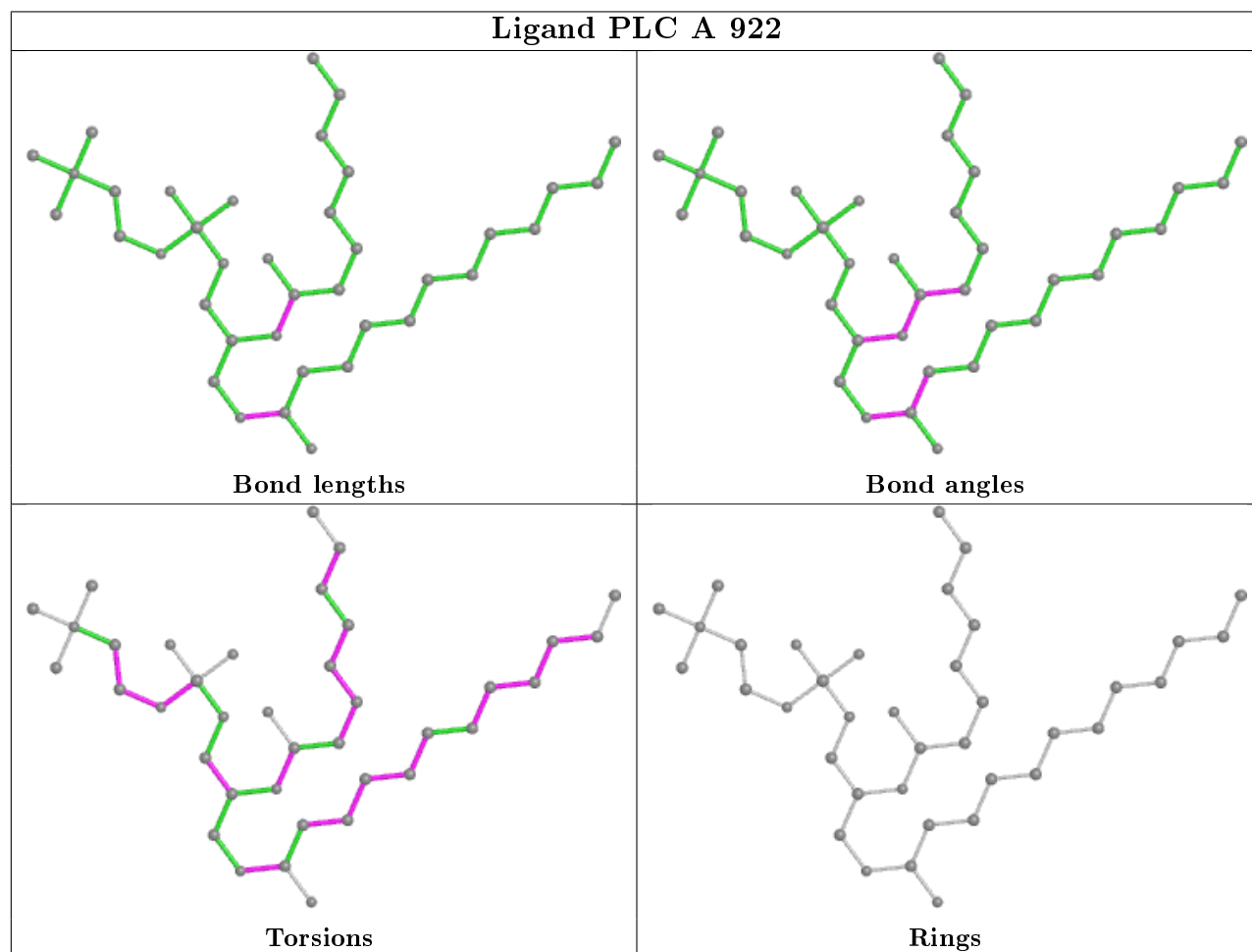
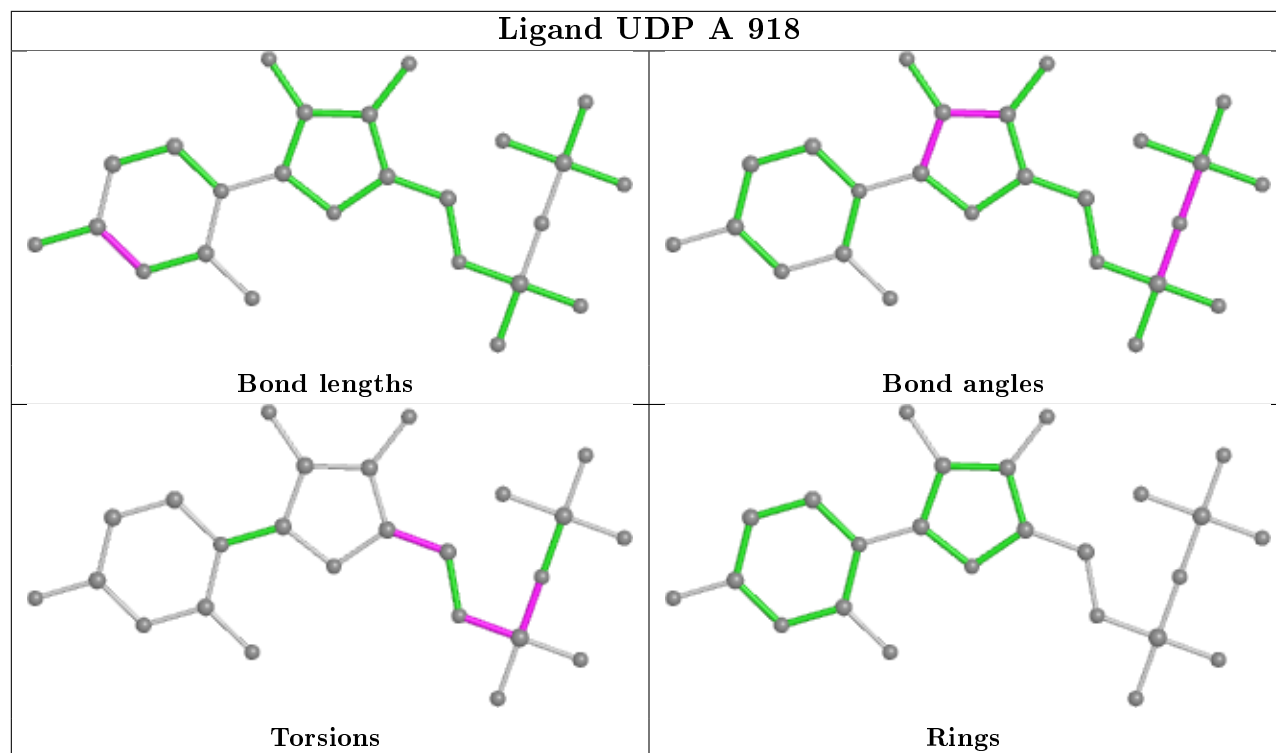
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	920	C2E	9	0
9	A	923	3PE	1	0
5	A	918	UDP	1	0
8	A	922	PLC	1	0
6	A	919	C2E	3	0

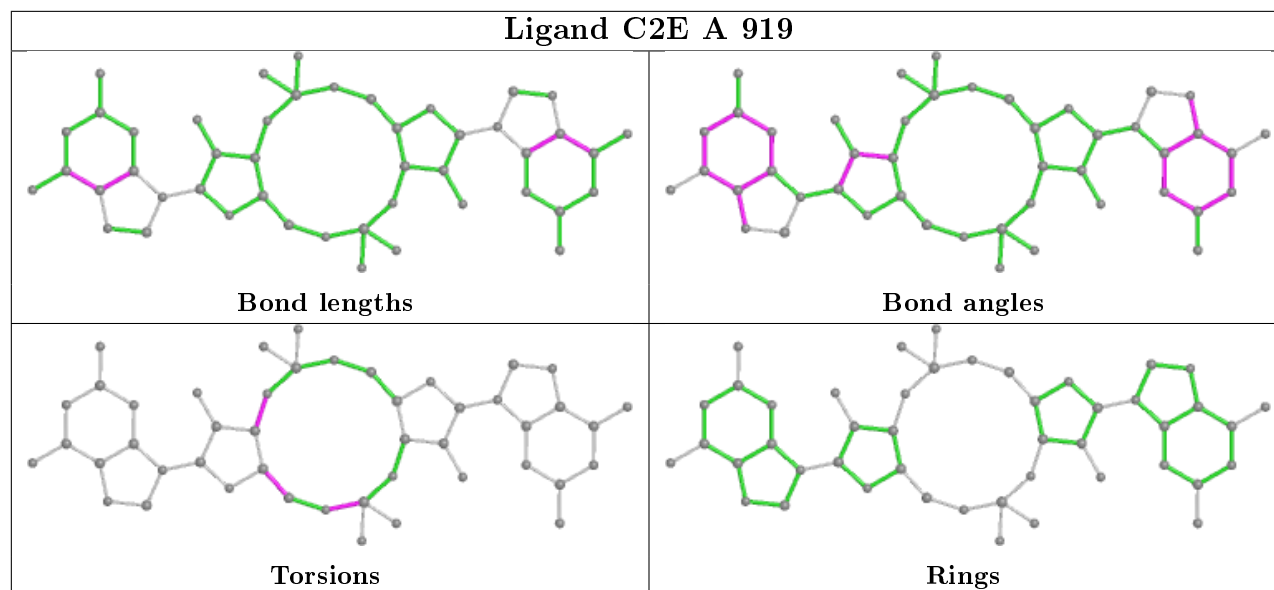
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the

average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	728/803 (90%)	-0.11	15 (2%) 63 49	45, 69, 116, 196	0
2	B	655/724 (90%)	-0.20	10 (1%) 73 61	42, 64, 112, 169	0
3	D	0/9	-	-	-	-
All	All	1383/1536 (90%)	-0.16	25 (1%) 68 55	42, 67, 115, 196	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	595	PRO	3.7
1	A	15	PRO	3.4
1	A	496	LEU	3.2
2	B	169	PHE	3.1
1	A	188	MET	3.0
2	B	593	LEU	3.0
2	B	168	GLU	2.8
2	B	592	MET	2.8
1	A	137	GLU	2.7
1	A	740	ARG	2.7
1	A	133	PRO	2.6
2	B	77[A]	GLN	2.4
2	B	596	GLY	2.4
2	B	589	VAL	2.3
1	A	16	VAL	2.3
1	A	221	ARG	2.2
1	A	190	PRO	2.2
1	A	136	PRO	2.2
1	A	192	PRO	2.2
1	A	13	VAL	2.2
2	B	78[A]	GLN	2.1
1	A	735	PRO	2.1
1	A	187	CYS	2.0

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Mol	Chain	Res	Type	RSRZ
2	B	494	ASP	2.0
1	A	223	GLU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

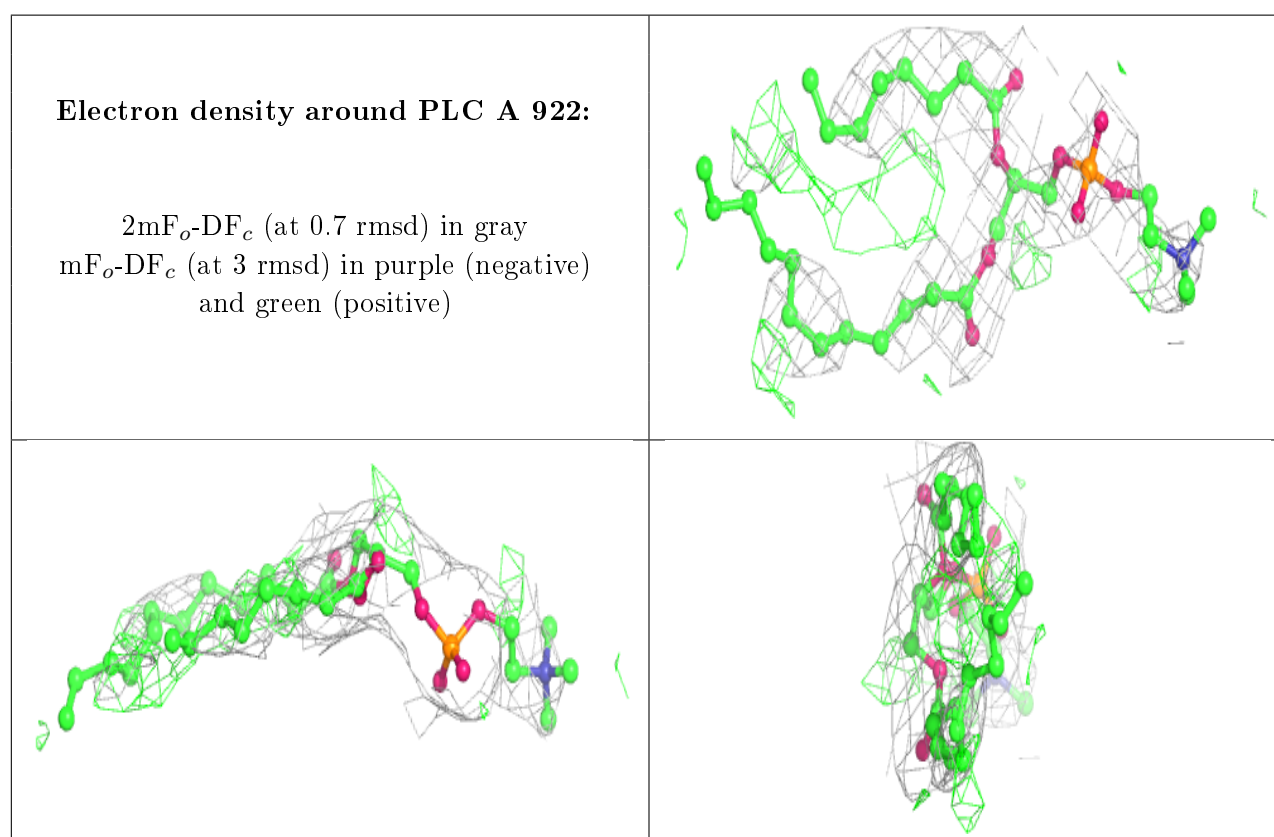
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	BGC	C	1	11/12	0.72	0.34	103,136,174,199	0
4	BGC	C	2	11/12	0.84	0.25	97,117,134,144	0
4	BGC	C	3	11/12	0.93	0.19	79,90,124,128	0
4	BGC	C	7	11/12	0.93	0.14	43,54,65,80	0
4	BGC	C	4	11/12	0.93	0.20	52,60,88,145	0
4	BGC	C	8	11/12	0.93	0.17	62,72,97,133	0
4	BGC	C	5	11/12	0.93	0.22	37,52,58,107	0
4	BGC	C	14	11/12	0.95	0.28	60,71,82,88	0
4	BGC	C	16	11/12	0.96	0.24	69,75,100,117	0
4	BGC	C	15	11/12	0.96	0.20	49,55,75,75	0
4	BGC	C	13	11/12	0.96	0.27	69,73,89,101	0
4	BGC	C	17	11/12	0.96	0.23	71,78,85,93	0
4	BGC	C	6	11/12	0.96	0.15	41,43,71,105	0
4	BGC	C	10	11/12	0.96	0.16	61,76,94,99	0
4	BGC	C	12	11/12	0.97	0.20	56,65,81,98	0
4	BGC	C	9	11/12	0.97	0.13	61,68,81,88	0
4	BGC	C	11	11/12	0.97	0.14	56,75,96,98	0

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

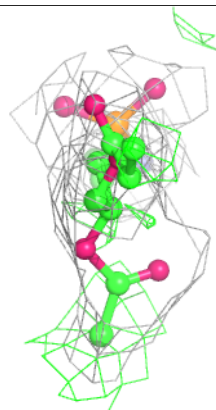
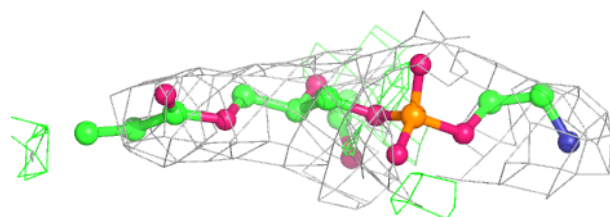
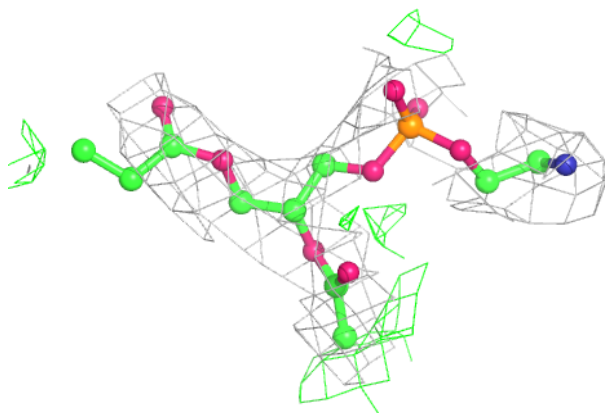
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
8	PLC	A	922	38/42	0.85	0.39	87,120,154,168	0
7	MG	A	921	1/1	0.89	0.41	36,36,36,36	0
9	3PE	A	923	20/51	0.90	0.22	71,90,113,120	0
5	UDP	A	918	25/25	0.92	0.23	54,80,92,126	0
6	C2E	A	920	46/46	0.97	0.11	35,56,70,91	0
6	C2E	A	919	46/46	0.97	0.12	31,51,63,76	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

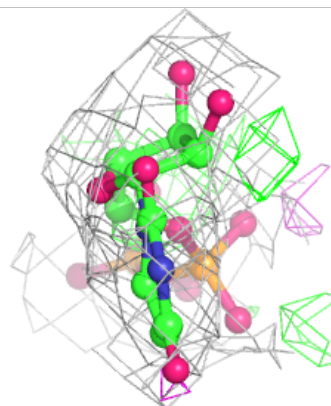
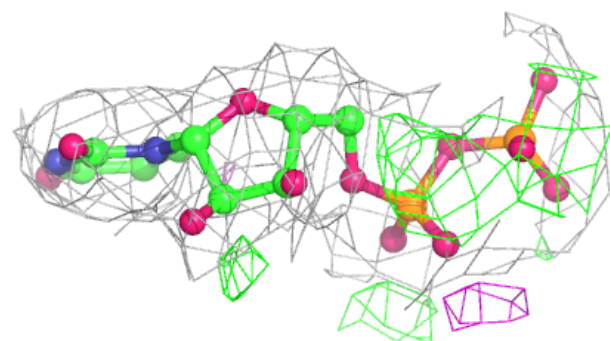
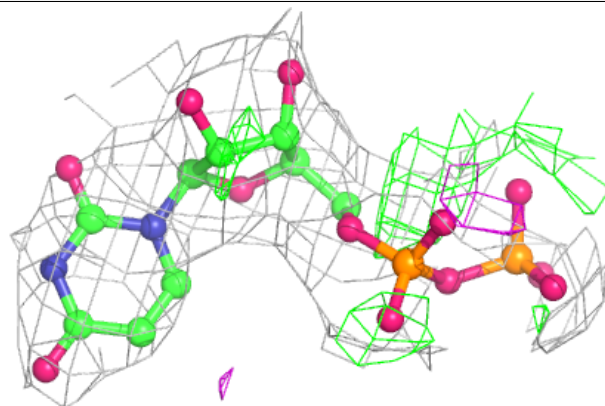


Electron density around 3PE A 923:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

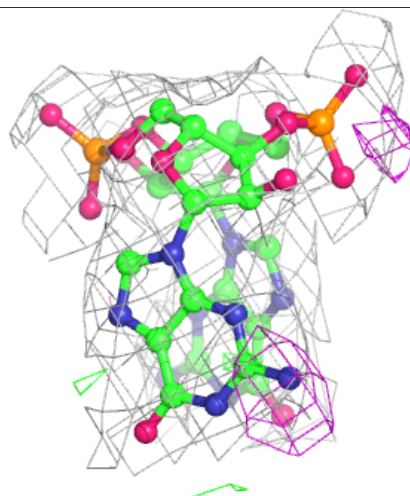
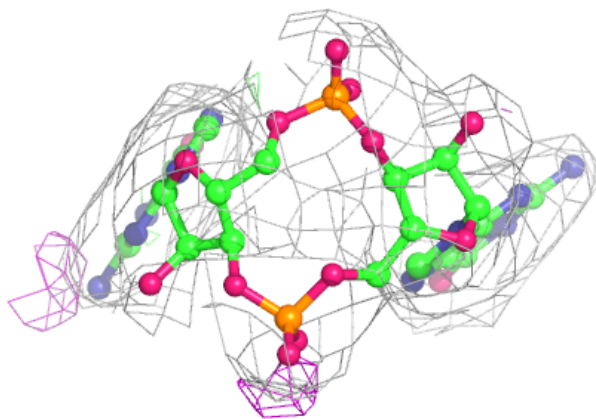
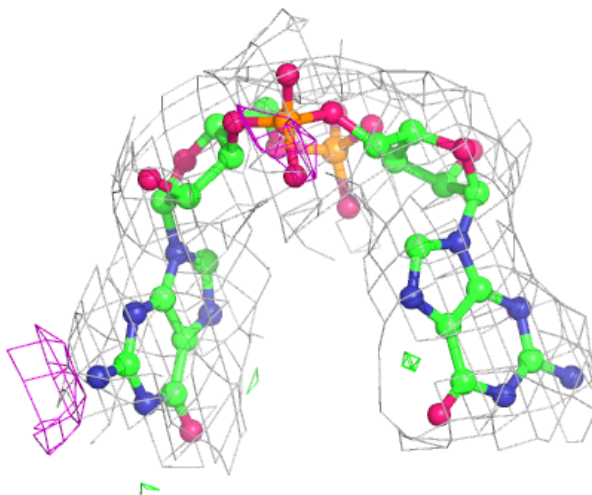
**Electron density around UDP A 918:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



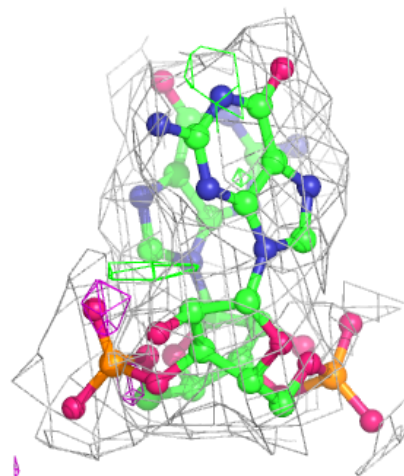
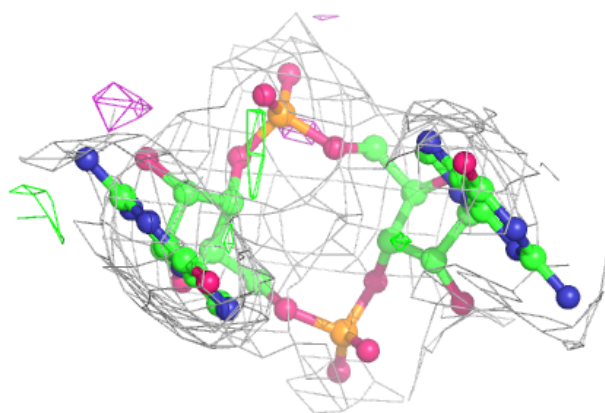
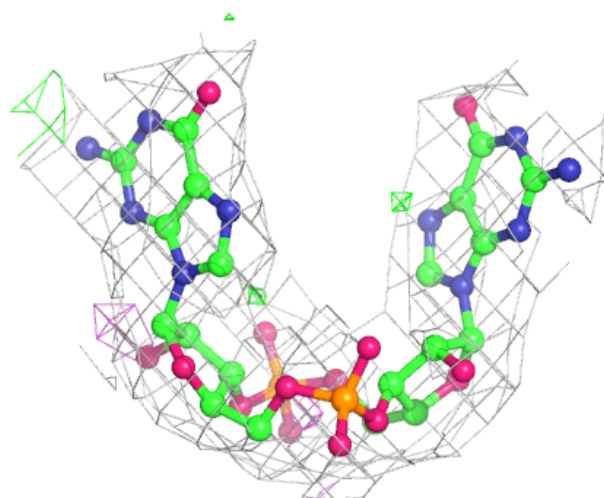
Electron density around C2E A 920:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around C2E A 919:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers ⓘ

There are no such residues in this entry.